

Code Club: Command Line

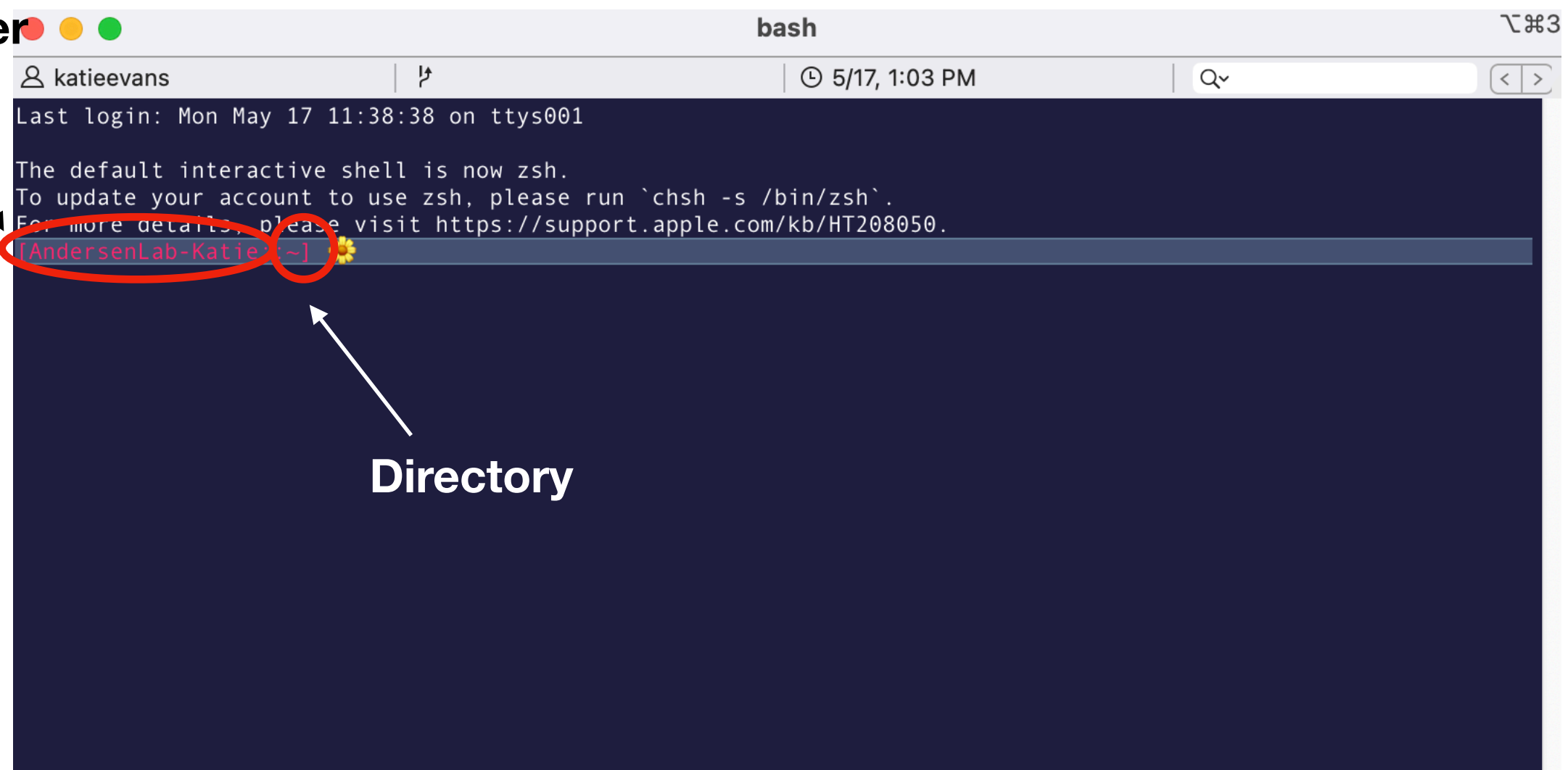
5.28.21

<http://andersenlab.org/dry-guide/latest/bash/>

Welcome to terminal!

Your command line!

Computer



The screenshot shows a macOS Terminal window titled "bash". The window has a title bar with red, yellow, and green window control buttons. The terminal content includes a login message for user "katieevans" on "ttys001", a notification about switching to the "zsh" shell, and a command prompt "[AndersenLab-Katie ~]". A red oval highlights the command prompt, and a white arrow points to it from the label "Directory".

```
bash
katieevans | 5/17, 1:03 PM
Last login: Mon May 17 11:38:38 on ttys001
The default interactive shell is now zsh.
To update your account to use zsh, please run `chsh -s /bin/zsh`.
For more details, please visit https://support.apple.com/kb/HT208050.
[AndersenLab-Katie ~]
```

Directory

On Mac: Terminal

Other 3rd party apps (like iTerm2 etc.)

Welcome to terminal!

Your command line!

```
ssh
kek973 | 5/17, 1:08 PM
Quest architectures and node specifications are below:
- quest5: 24 cores & 128 GB memory per node
- quest6: 28 cores & 128 GB memory per node
- quest8: 28 cores & 96 GB memory per node
- quest9: 40 cores & 192 GB memory per node
- quest10: 52 cores & 192 GB memory per node

On Quest's login nodes, users cannot request more than 4 cores and/or 4 GB of memory in total for all commands and code they are running.

Please remember that Quest is not approved for contractually or legally restricted data. Ensure sensitive data is anonymized or de-identified before being moved to Quest. Contact us if you need a computing environment for the use of restricted data.

Information on Quest can be found at http://www.it.northwestern.edu/research/user-services/quest/index.html.

Quest enforces memory limits on jobs. For more information, please see https://kb.northwestern.edu/specifying-memory-for-jobs-on-quest.

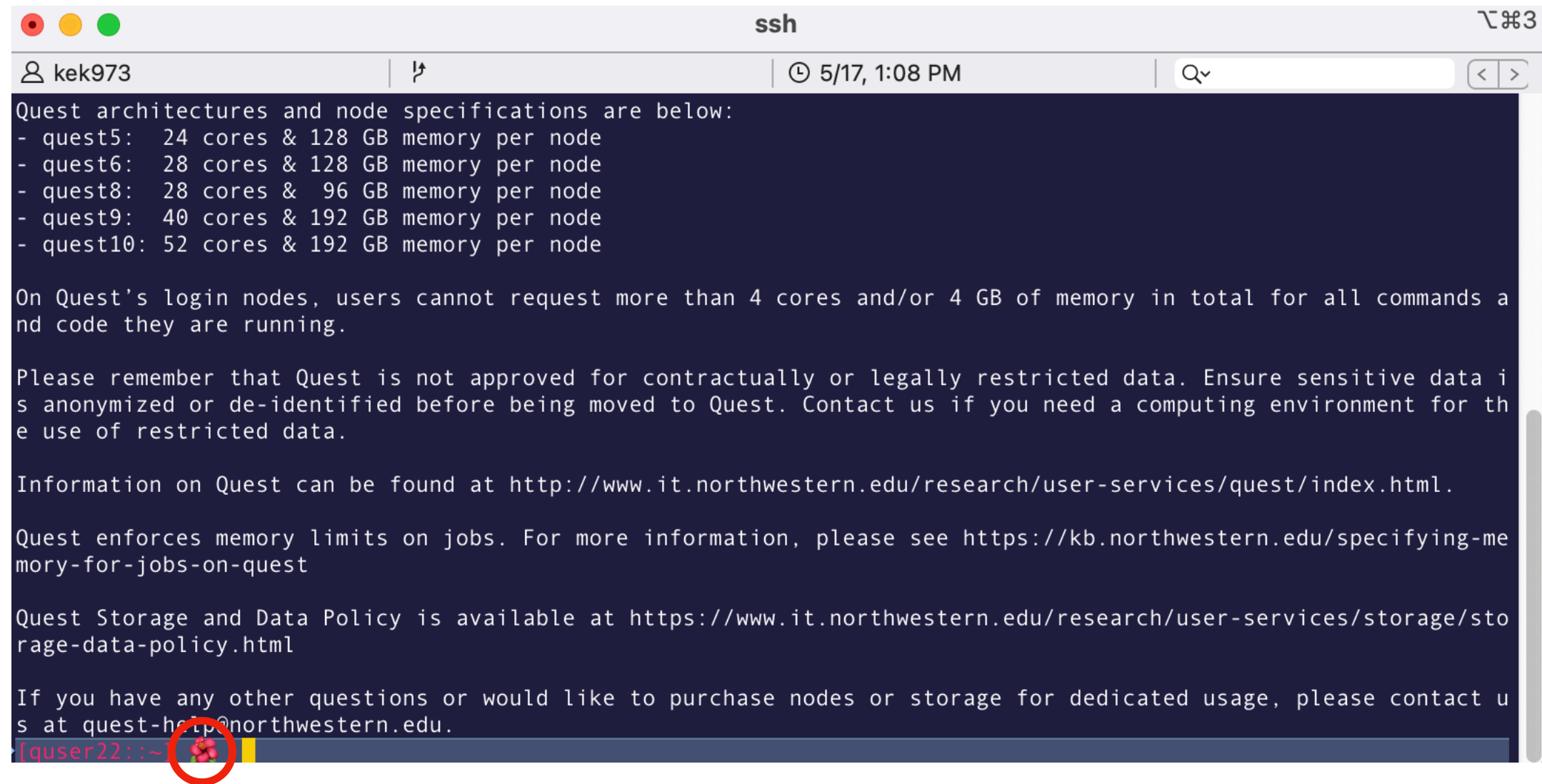
Quest Storage and Data Policy is available at https://www.it.northwestern.edu/research/user-services/storage/storage-data-policy.html.

If you have any other questions or would like to purchase nodes or storage for dedicated usage, please contact us at quest-help@northwestern.edu.
[quser22 ~]
```

On Mac: Terminal

Other 3rd party apps (like iTerm2 etc.)

Welcome to terminal!



The screenshot shows an SSH terminal window titled 'ssh' with a user 'kek973'. The terminal displays the following text:

```
Quest architectures and node specifications are below:
- quest5: 24 cores & 128 GB memory per node
- quest6: 28 cores & 128 GB memory per node
- quest8: 28 cores & 96 GB memory per node
- quest9: 40 cores & 192 GB memory per node
- quest10: 52 cores & 192 GB memory per node

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[user22:~] 
```

The prompt '[user22:~]' is highlighted with a red circle, and a flower icon is visible next to it.

```
vi ~/.bash_profile
```

Cool prompt generator!!!

```
export PS1=' \[\e[0;35m\][\h::\W]  \[\e[m\] '
```

This stuff also determines the colors and what is shown on the prompt

Welcome to terminal!

New terminal tab

Command + T

New terminal window

Command + N

Show previous command

Up arrow

```
~/.bash_profile
```

```
alias quest="ssh <netid>@quest.northwestern.edu"
```

> quest  Logs in to quest using ssh ^

Log in to QUEST

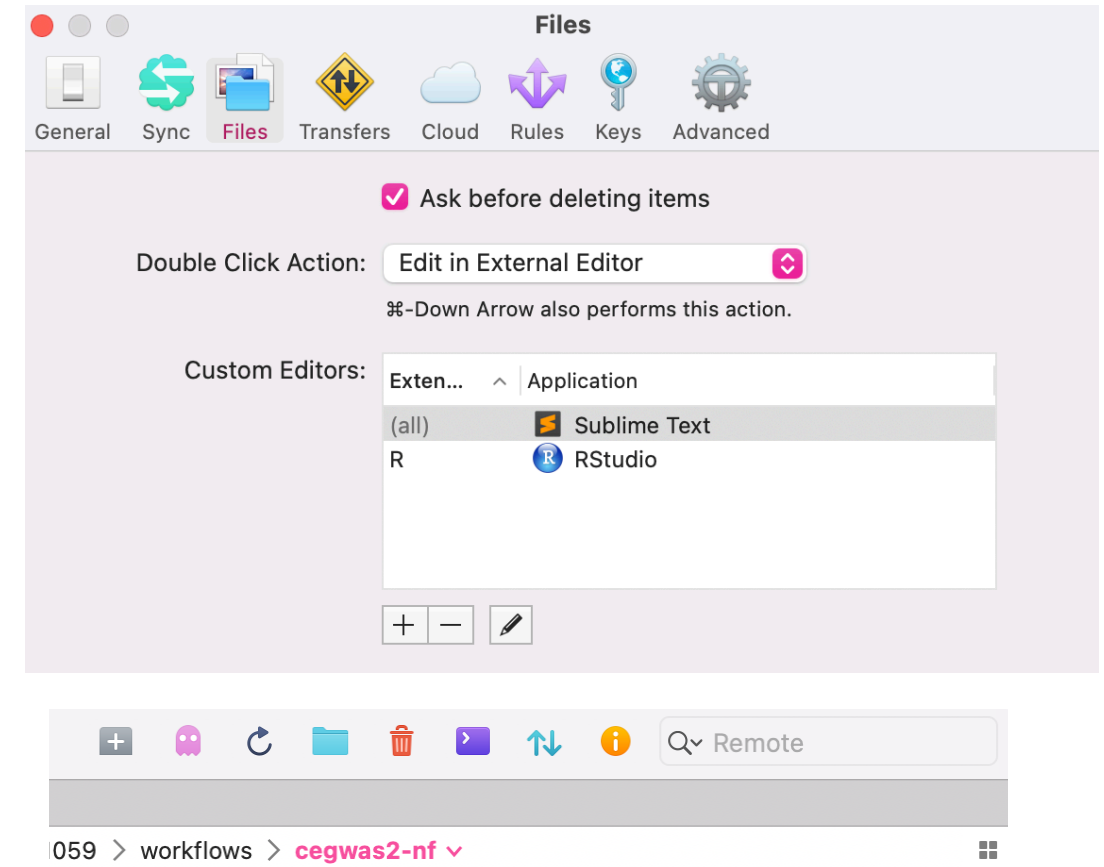
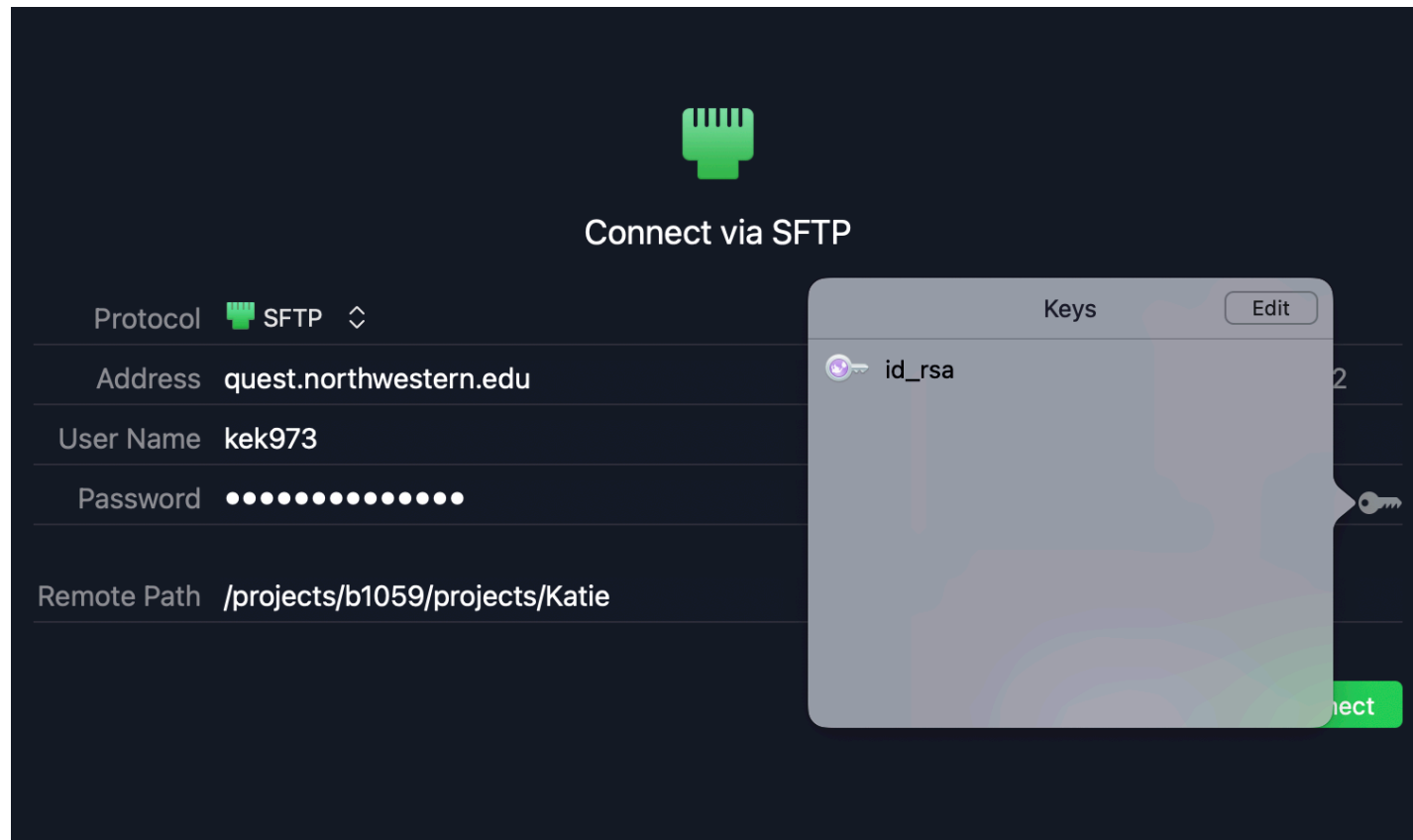
```
{ ssh <netid>@quest.it.northwestern.edu }  
{ ssh <netid>@quest.northwestern.edu }
```

(Enter password when prompted)

(Set up ssh key to avoid typing password each time):

LOCAL	<pre>cd ~ ssh-keygen (keep default name, overwrite it if asks, no password needed, just press ENTER) cat ~/.ssh/id_rsa.pub (copy entire output)</pre>
QUEST	<pre>cd ~/.ssh (or make directory if new) vi authorized_keys (paste contents from id_rs.pub, save, exit)</pre>

Transmit/CyberDuck etc.



```
scp <netid>@quest.northwestern.edu:<path_on_quest>/file.txt .
```

```
scp file.txt <netid>@quest.northwestern.edu:<path_on_quest>
```

Terminal alternatives



<https://iterm2.com/>

<https://www.fossmint.com/alternative-terminal-apps-for-macos/>

Introduction to the basics

Change directories (hard path)

```
cd ~/Dropbox/AndersenLab/LabFolders/Katie/
```

Don't forget
about TAB
completion :)

Change directories (relative path)

```
cd ../Clay/
```

Print current directory

```
pwd
```

Create new directory

```
mkdir new_folder
```

Create new file

```
touch new_file.tsv
```

Introduction to the basics

**Be careful
with this one!!
You WILL
overwrite if
the file already
exists. Also
try:**

`mv -i new_file.tsv ../Tim`

Move a file

`mv new_file.tsv ../Tim/`

Move (and rename) a file

`mv new_file.tsv ../Tim/new_file2.tsv`

Rename a file (without moving)

`mv new_file.tsv ./new_file2.tsv`

Copy a file

`cp new_file.tsv new_file_copy.tsv`

Open a file

`open new_file.tsv`

Introduction to the basics

List files in a directory

`ls` `ls ~/Dropbox/AndersenLab`

List files with more information about the files

`ls -l` `ls -ltr` `ls -lah` (man `ls`) for more options

Delete a file

`rm new_file.tsv`

Delete an empty folder

`rmdir new_folder`

****Delete a full folder (and all files inside)****

`rm -r new_folder`

**Be careful
with this one!!
Once deleted,
it's gone! Use
at your own
risk**

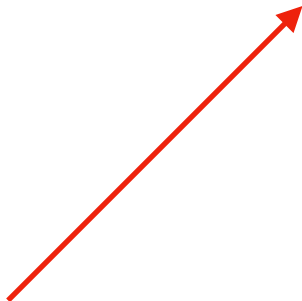
`rm -i new_file.tsv`

Introduction to the basics

Create file using redirection

```
ls ~/Dropbox/AndersenLab/LabFolders > people.txt
```

**Be careful
with this one!!
You WILL
overwrite
previous
“people.txt”
with this
command**



Print the contents of a file

```
cat people.txt
```

Print a line of text or string

```
echo "this is a test"
```

Add a new line to an existing file

```
echo "Alyssa" >> people.txt
```

Concatenate (put together) multiple files

```
cat file1.txt file2.txt
```

Introduction to the basics

View contents of a file

`more file.txt`

`less file.txt`

Find/search for a file

`find <directory> -name "file.txt"`

Pipe commands together (like %>%)

`cat file.txt | head`

Download file from url

`wget <url>`

`wget -bqc <url>`

`curl <url>`

Pull out lines with pattern

`cat file.txt | grep ECA1242`

Scroll up/down
Use **q** to exit

OR:

`ls -R * | grep ECA1119`

**less is similar
to more, but
faster because
it does not
load the entire
file at once**

**Download in
background**

**Highlight all
mention of
"ECA1242"**

Introduction to the basics

Count words in a file

```
wc file.txt
```

Count lines in a file

```
wc -l file.txt
```

Count number of files in directory

```
ls -ltr | wc -l
```

Print the first few (n) lines of a file

```
head file.txt
```

```
head -n 20 file.txt
```

Print the last few (n) lines of a file

```
tail file.txt
```

Introduction to the basics

Set a variable

```
chr="V"; echo $chr
```

Sort lines in a file

```
head test.tsv | sort -k7
```


Sort by 7th col



Get unique values

```
head test.tsv | awk '{print $7}' | uniq
```

Can only find
unique lines
next to each
other, might
need to **sort**
first



Intermediate tasks

~ If/else - BASH ~

```
if [[logical]]
then
    [commands]
else
    [commands]
fi
```

```
if [[ $sp == "ce" ]]
then
    echo "TRUE"
else
    echo "FALSE"
fi
```

```
if [[ $sp == "ce" ]]; then echo "TRUE"; else echo "FALSE"; fi
```

~ If/else - R ~

```
if(logical) {
    [commands]
} else {
    [commands]
}
```

```
if(species == "c_elegans") {
    print("TRUE")
} else {
    print("FALSE")
}
```


Intermediate tasks

~ For loop - BASH ~

```
for item in [LIST]
do
    [commands]
done
```

```
for base in A C G T
do
    echo "Base: $base"
done
```

~ For loop - R ~

```
for(item in [LIST] {
    [commands]
}
```

```
for(base in c("A", "C", "G", "T")){
    print(paste("Base:", base))
}
```

```
for base in A C G T; do echo "Base: $base"; done
```

Intermediate tasks

~ For loop - BASH ~

```
for item in [LIST]
do
    [commands]
done
```

```
for file in `ls`
do
    echo $file
done
```

Use `` to implement code in a command

Intermediate tasks

bash_script.sh

```
#!/bin/bash
#SBATCH -J name           # Name of job
#SBATCH -A b1042          # Allocation
#SBATCH -p genomicsguestA # Queue
#SBATCH -t 24:00:00       # Walltime/duration of the job (hh:mm:ss)
#SBATCH --cpus-per-task=1  # Number of cores (= processors = cpus) for each task
#SBATCH --mem-per-cpu=3G   # Memory per core needed for a job
#SBATCH --array=0-9        # number of parallel jobs to run counting from 0. Make sure to c

# make a list of all the files you want to process
# this script will run a parallel process for each file in this list
name_list=(*.bam)

# take the nth ($SGE_TASK_ID-th) file in name_list
# don't change this line
Input=${name_list[$SLURM_ARRAY_TASK_ID]}

# then do your operation on this file
Output=`echo $Input | sed 's/.bam/.sam/'`
```

sbatch bash_script.sh

squeue -u <netid>

scancel <jobid>

Intermediate: Screen/nohup

Perhaps the most common way to deal with scripts that run for a long time is `screen`. For the most simple case use, type `screen` to open a new screen session and then run your script like normal. Below are some more intermediate commands for taking full advantage of `screen`:

- `screen -S <some_descriptive_name>`: Use this command to name your screen session. Especially useful if you have several screen sessions running and/or want to get back to this particular one later.
- `Ctrl+a` + `Ctrl+d` to detach from the current screen session
- `exit` to end the current screen session
- `screen -ls` lists the IDs of all screen sessions currently running
- `screen -r <screen_id>`: Use this command to resume a particular screen session. If you only have one session running you can simply use `screen -r`

Important

When using `screen` on QUEST, take note that screen sessions are only visible/available when you are logged on to the particular node it was created on. You can jump between nodes by simply typing `ssh` and the login node you want (e.g. `ssh quser22`).

Intermediate: Screen/nohup

Another way to avoid **SIGHUP** errors is to use `nohup`. `nohup` is very simple to use, simply type `nohup` before your normal command and that's it!

```
nohup nextflow run main.nf
```

Running a command with `nohup` will look a little different than usual because it will not print anything to the console. Instead, it prints all console outputs into a file in the current directory called `nohup.out`. You can redirect the output to another filename using:

```
nohup nextflow run main.nf > cegwas_{date}_output.txt
```

When you exit this window and open a new session, you can always look at the contents of the output file using `cat nohup.out` to see the progress.

Note

You can also run `nohup` in the background to continue using the same window for other processes by running `nohup nextflow run main.nf &`.

Intermediate: Software/conda

Modules

- `module avail` # what Quest has
- `module list` # what I have loaded
- `module add/load` # load a module
- `module purge` # remove all modules

Conda

- `module load python/anaconda`
- `conda create -n name_env` # create environment
- `conda activate name_env` # go inside the env
 `source activate name_env` # if the line above doesn't work
- `conda install -c bioconda nextflow=0.20.0`
 `conda install nextflow` # if .condarc is set up
- `conda deactivate` # go inside the env
 `source deactivate` # if the line above doesn't work

Intermediate: Software/conda

	benefits	limitations
Manual install	<ul style="list-style-type: none">- Full control by users	<ul style="list-style-type: none">- May fail- Less easy to turn on and off
Modules	<ul style="list-style-type: none">- Easiest to use	<ul style="list-style-type: none">- Not managed by users- Don't know what's in there or what changes
Conda	<ul style="list-style-type: none">- Easy to use- Easy to share and reproduce- Bundles of packages	<ul style="list-style-type: none">- Still sees the other packages
Docker/ Singularity	<ul style="list-style-type: none">- Fully isolated environment- Highly portable	<ul style="list-style-type: none">- Takes a bit more work to set up

Advanced: bcftools

- **annotate** .. edit VCF files, add or remove annotations
- **call** .. SNP/indel calling (former "view")
- **cnv** .. Copy Number Variation caller
- **concat** .. concatenate VCF/BCF files from the same set of samples
- **consensus** .. create consensus sequence by applying VCF variants
- **convert** .. convert VCF/BCF to other formats and back
- **csq** .. haplotype aware consequence caller
- **filter** .. filter VCF/BCF files using fixed thresholds
- **gtcheck** .. check sample concordance, detect sample swaps and contamination
- **index** .. index VCF/BCF
- **isec** .. intersections of VCF/BCF files
- **merge** .. merge VCF/BCF files from non-overlapping sample sets
- **mpileup** .. multi-way pileup producing genotype likelihoods
- **norm** .. normalize indels
- **plugin** .. run user-defined plugin
- **polysomy** .. detect contaminations and whole-chromosome aberrations
- **query** .. transform VCF/BCF into user-defined formats
- **reheader** .. modify VCF/BCF header, change sample names
- **roh** .. identify runs of homo/auto-zygosity
- **sort** .. sort VCF/BCF files
- **stats** .. produce VCF/BCF stats (former vcfcheck)
- **view** .. subset, filter and convert VCF and BCF files

Advanced: bcftools

Do you have bcftools??

```
module load bcftools
```

View VCF

```
bcftools view <vcf>
```

View VCF only header (-h) or without header (-H)

```
bcftools view -h <vcf>
```

```
bcftools view -H <vcf>
```

Subset vcf for only 3 samples

```
bcftools view -s CB4856,XZ1516 <vcf>
```

Subset vcf for a region of interest

```
bcftools view -r III:1-800000 <vcf>
```

Advanced: bcftools

Print out contents of vcf in a specific format

```
bcftools query -f '%CHROM\t%POS\t%REF\t%ALT[\t%SAMPLE=%GT]\n' <vcf> >  
out.tsv
```

Print list of samples in vcf

```
bcftools query -l <vcf>
```

Keep rows that include a tag (i.e. filter?)

```
bcftools query -i GT=="alt" <vcf>
```

Remove rows that include a tag

```
Bcftools query -e GT=="ref" <vcf>
```

[Bcftools manual](#)

[Bcftools cheat sheet](#)

Advanced: awk

- 'awk' is a utility/language designed for **data extraction**
- Often used in combination with **sed**
- Reads one line at a time
- syntax: **awk 'condition {action}'**
- Awk guide, **examples**

Advanced: awk

Print only columns 1 and 3 using stdin

```
awk '{print $1,$3}'
```

\$1 = 1st column/field

\$0 = all cols

NF = number of fields

\$NF = last col

\$(NF-1) = second to last

Print elements from column 2 that match a pattern using stdin (filter)

```
awk '/HIGH/ {print $6}'
```

regex is specified within //

Create new column

```
echo 'foo,bar,123,baz' | awk -F, -v OFS=, '{ $5=42 } 1'
```

```
awk 'BEGIN { FS = OFS = "\t" } { $(NF+1) = 1; print $0 }' infile
```

Prints every record between 2405089 and 3729798 (2nd col)

```
awk '$2 == 2405089, $2 == 3729798' test.tsv
```

Advanced: awk

Use a different delimiter

```
echo 'foo:123:bar:789' | awk -F':' '{print $2}'
```

Split with regular expressions

```
echo 'Sample123string54with908numbers' | awk -F'[0-9]+' '{print $2}'
```

Change csv to tsv

```
echo 'foo,123,bar,789' | awk -F',' -v OFS='\t' '{$1=$1; print $0}'
```

```
echo 'foo,123,bar,789' | awk '{gsub(",", "\t")}' 1'
```

Print every line except header

```
awk 'NR>1' inputfile.tsv
```

Advanced: awk

Print header and lines (columns 1 and 2) where position < 3000

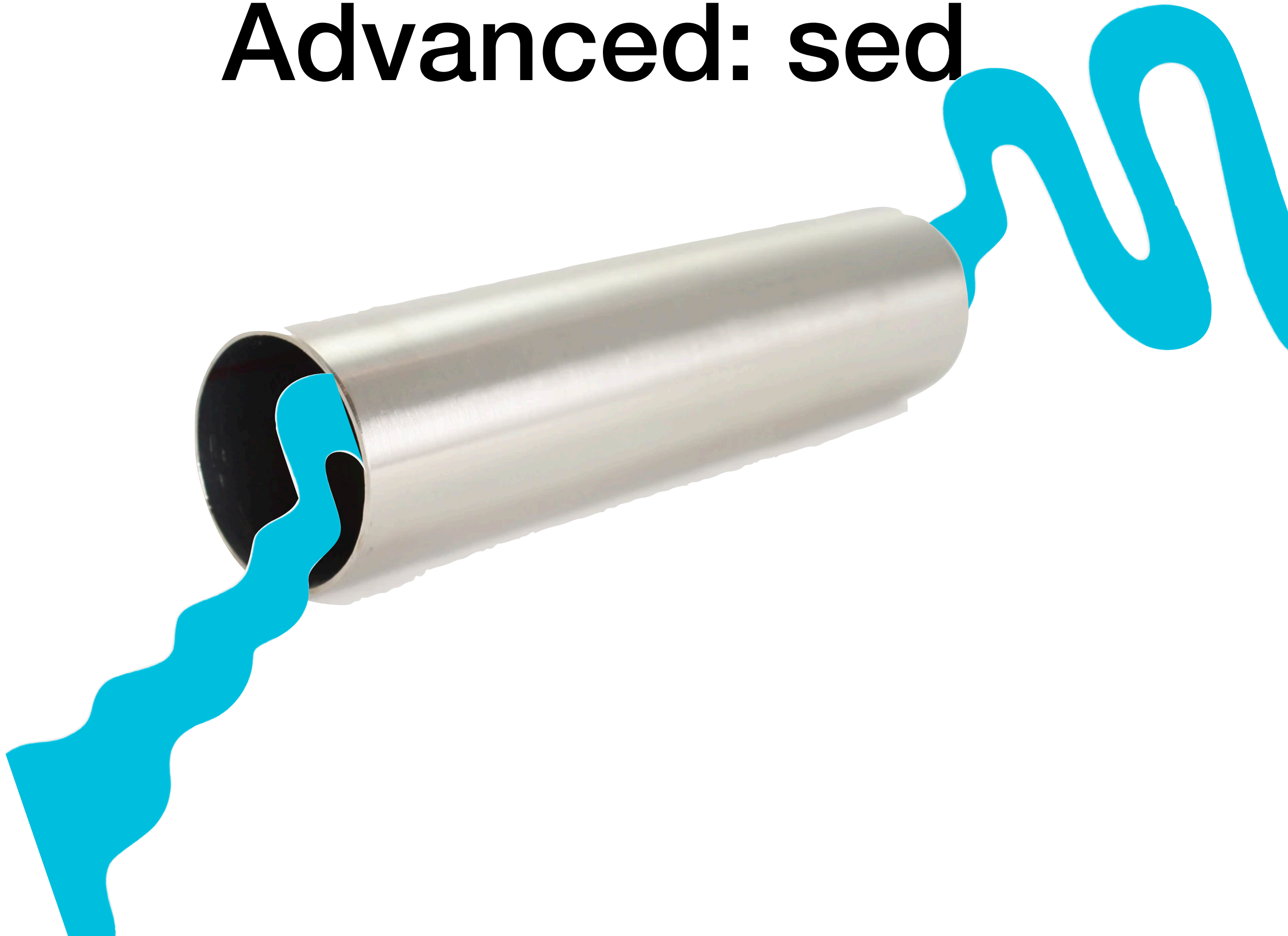
```
awk 'NR==1 || $2<3000 {print $1,$2}' inputfile.tsv
```



```
Awk '{
    if(NR==1 || $2<3000){
        print $1,$2
    }
}' inputfile.tsv
```

SO SO SO SO MUCH MORE (I know nothing...)

Advanced: sed



Advanced: sed

Essential command: s for substitution

```
sed s/pattern/replacement/ input > output
```

```
echo 'C. elegans is amazing!' | sed 's/elegans/briggsae/'
```

Doesn't need
quotes, but good
practice



Think about the substitutions you are asking it to make...

```
echo 'Sunday funday' | sed 's/day/night/'
```

Default behavior is to replace once per line... to change that, use 'g'

```
echo 'Sunday funday' | sed 's/day/night/g'
```